DEVELOPMENT OF A PHYSICALLY-BASED METHODOLOGY FOR PREDICTING MATERIAL VARIABILITY IN FATIGUE CRACK INITIATION AND GROWTH RESPONSE

Final Report
SwRI® Project No. 18.05010

by
Kwai S. Chan

AFOSR FINAL REPORT

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Air Force Research Laboratory
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December 2004

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The report summarizes the results of an interdisciplinary program aimed at developing a computational methodology for treat material variability in the fatigue crack initiation and growth responses of aerospace structural alloys. In this three-year program, physics-based fatigue crack initiation and growth models were developed and integrated into a probabilistic micromechanical code for treating fatigue life variability resulting from material variations. Dubbed MicroFaVa (**Micro**mechanical **Fa**tigue **Va**riability), the code is based on a set of physics-based fatigue models that predict fatigue crack initiation life, fatigue crack growth life, fatigue limit, fatigue crack growth threshold, crack size at initiation, and fracture toughness. Using microstructure information as material input, the code is capable of predicting the average behavior and the confidence limits of the crack initiation and crack growth lives of structural alloys under LCF or HCF loading. The code has been integrated and utilized with DARWIN®, a probabilistic design and life-prediction code developed at Southwest Research Institute (SwRI®), to treat fatigue life variability in a Ti rotor due to variation in the microstructure. The probabilistic micromechanics code has been verified and validated against two benchmark problems with known solutions, as well as comparisons against an extensive database of fatigue life and fatigue crack growth data.

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PREFACE

DISCLAIMER

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EXECUTIVE SUMMARY

The main objective of this basic research program was to develop a generic physics-based computational methodology for accurately predict the fatigue properties of structural alloys and their variability with microstructure. The objective of the program was achieved in three tasks with these aims: (1) to develop physically based fatigue crack initiation and growth models, (2) to develop a probabilistic approach for linking physically based models into a continuum framework, and (3) to demonstrate the utilities of the methodology in a probabilistic design setting

An integrated interdisciplinary modeling/experimental approach involving a combination of materials sciences, micromechanics, and probabilistic techniques was used to develop a suite of physically-based models for describing dislocation structure evolution, fatigue crack initiation, fatigue crack growth (FCG) and threshold behaviors, as well as the linkage of these processes over the atomistic, dislocation cell, grain, and continuum size scales. This set of fatigue models was incorporated into a probabilistic framework and integrated into a computer code named MicroFaVa (Micromechanical Fatigue Variability Code) for predicting fatigue properties and life variability due to material variation. The probabilistic material code was coupled to and utilized with DARWIN®, a probabilistic design and life-prediction code developed at Southwest Research Institute (SwRI®), to treat fatigue life variability in a Ti rotor due to variation in the microstructure.

The key accomplishments of this program are (1) the development of physically-based fatigue crack initiation and growth models; (2) the development of a probabilistic code named MicroFaVa for treating fatigue life variability resulting from material variation; (3) the incorporation of MiCroFaVa with a probabilistic design code DARWIN® and their application in the life prediction for a structural component made of Ti-6Al-4V; (4) an extensive and systematic assessment of the predictive capability of the physics-based fatigue models; and (5) verification and validation of the integrated probabilistic design and lifing methodology by applying the computational approach to two benchmark problems with known solutions. In addition, the utility of the computed material input was successfully demonstrated by one to one comparisons against the conventional method based on empirical data input. The probabilistic micromechanical code was utilized to elucidate the influence of microstructural variation on the propagation and arrest of grain-sized small cracks, the probability density function of small-crack thresholds, as well as the occurrence of dual fatigue limits for crack initiation and growth. These computational results were used to develop fundamental understandings on pertinent microstructure/fatigue resistance relationships such as: (i) the dependence of the intrinsic threshold on the planarity of slip and dislocation cell formation, (iii) the occurrence of dual fatigue thresholds and dual fatigue limits resulting from differences in fatigue mechanisms, (iii) fatigue life variation resulting from difference in the slip morphology and enhanced fatigue crack initiation life by dislocation cell formation, and (iv) dependence of FCG rate on dislocation density at the crack tip. Most of these results are published in the open literature or have been submitted for publication.

The technology developed in this program has been incorporated into DARWIN® and transferred to the USAF DUST program (Contract No. F33615-03-2-5203) at SwRI. The probabilistic micromechanics-based life methodology is in the process of being transferred to a DARPA-supported program entitled "A Revolutionary Smart Materials Approach to Structural Health Monitoring and Progress" (Contract No. HR0011-04-0004) at SwRI and an AFOSR program on Vehicle Health Monitoring (Contract No. FA95500410254) at University of Texas at San Antonio.

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1.0 INTRODUCTION

There is a need to develop affordable new materials by reducing the long lead time and the number of material and processing iterations required to achieve the desired material properties. Traditional approaches based on trails and errors used in material development need to be replaced with computer-assisted, science-based approaches so the desired mechanical properties can be achieved in new materials systematically, efficiently, and affordably. Thus, there is a need for a generic physics-based computational methodology that accurately predicts the mechanical properties of new materials and their microstructure so that computer-assisted optimization procedure can be applied to obtain the desired microstructures and mechanical properties.

Fatigue crack growth properties of structural alloys generally exhibit variability because of variations in microstructure. This variability is traditionally characterized by extensive testing to develop a large database so that the mean, variance, and the lower bound of the fatigue properties can be ascertained. An obvious drawback of this approach is that an experimental database is time-consuming and costly to generate. Another limitation is that the empirical approach seldom provides information regarding the sensitivities of various material parameters to the probability of fracture associated with a particular component or the means for reducing fatigue variability. One of the contributing factors to this problem is that most existing fatigue life or crack growth models are not linked with the fundamental material parameters; instead they are based on empirical constants obtained from curve fits of data from physical tests. Although these models characterize the main descriptors (mean, variance) of fatigue life as a function of applied stress range (S-N_f curves) or fatigue crack growth rate, da/dN, as a function of stress intensity factor range, ΔK, they provide little or no physical insight into the material parameters that influence failure associated with fatigue crack nucleation and growth.

In general, fatigue life can generally be considered to consist of two parts, which are crack initiation and crack propagation lives. The crack propagation life, N_f, can be predicted by integrating the da/dN equation, leading to

$$N_{\mathrm{f}} = \int_{a_i}^{a_{\mathrm{f}}} \left[\frac{da}{dN} \right]^{-1} da \tag{1}$$

where a_i and a_f are the initial and final crack length, respectively, and a_f is defined as the critical crack length at fracture. The fatigue crack growth (FCG) life, N_f, is most sensitive to the initial crack size, a_i [1], but also depends on microstructure, which can alter intrinsic material properties as well as extrinsic properties originating from crack shielding mechanisms.

As a result, a physics–based computational methodology required to address the effects of microstructure variation on fatigue life variability must include: (1) a microstructure-based crack initiation model for predicting initiation life and initial crack size distribution, (2) a microstructure-based fatigue crack growth model, and (3) a probabilistic framework for treating random material variables in the fatigue models and for probabilistic design and life assessment of structural components. This report describes the result of a basic research program to develop a generic physics-based computational methodology for predicting fatigue life response of structural alloys and their variability with microstructure.

2.0 PROGRAM OBJECTIVES AND APPROACH

2.1 Research Objectives

The main objective of this basic research program was to develop a generic physics-based computational methodology for accurately predict the fatigue properties of structural alloys and their variability with microstructure. The objective of the program was achieved in three tasks with these aims: (1) to develop physically based fatigue crack initiation and growth models, (2) to develop a probabilistic approach for linking physically based models into a continuum framework and a generic physics-based computational code for predicting fatigue life properties and variability in structural alloys, and (3) to demonstrate the utilities of the methodology in a probabilistic design setting.

2.2 Approach

An integrated interdisciplinary modeling/experimental approach involving a combination of materials sciences, micromechanics, and probabilistic techniques was used to develop a suite of physically-based models for describing dislocation structure evolution, fatigue crack initiation, fatigue crack growth (FCG) and threshold behaviors, as well as the linkage of these processes over the atomistic, dislocation cell, grain, and continuum size scales.

3.0 SUMMARY OF KEY RESULTS

The key results of this program are (1) the development of physically-based fatigue crack initiation and growth models, (2) the development of a probabilistic code named MicroFaVa for treating fatigue life variability resulting from material variation, and (3) the incorporation of MiCroFaVa with a probabilistic design code DARWIN and their application in the life prediction for a structural component made of Ti-6Al-4V. In this report, a brief summary of the probabilistic fatigue crack initiation and growth models in MicroFaVa is first presented. Second, the application of the probabilistic model to predicting the FCG variability in Ti-6Al-4V is highlighted. Finally, application of the model to lifing a Ti rotor design is demonstrated.

3.1 Probabilistic Fatigue Crack Growth Rate Modeling

The physics-based crack growth model proposed by Chan and Enright for treating the three stages of fatigue crack growth has the form given by [5, 6, 7]:

$$\frac{da}{dN} = \frac{2s\xi^{n_2/2}}{\left[E(2s)^{1/2}\right]^{n_2}}\left[\Delta K_T^{n_1-n_2}\Delta K_{eff}^{-n_1} + \Delta K_{eff}^{-n_2} - \left[(1-R)K_c\right]^{-n_2}\right]^{-1} \tag{2}$$

with

$$\xi = \frac{Es}{4\sigma'_y \varepsilon'_f \, d} \tag{3}$$

$$d = d_o\left(\frac{D}{D_o}\right)^{\gamma} \tag{4}$$

and

$$\Delta K_T = \frac{\Delta\sigma'_y}{\Delta\sigma_e}\Delta K_{th} \tag{5}$$

where the fatigue crack growth rate, *da/dN*, is expressed in terms of an effective stress intensity range, ΔK_{eff}, which is the difference between the applied stress intensity range, ΔK, and the stress intensity range at crack closure, ΔK_{cl}; ξ, a dimensionless normalizing parameter defined in terms of the Young's modulus (E), dislocation cell size (s), cyclic yield stress (σ'_y), fatigue ductility coefficient (ε'_f), and the dislocation barrier spacing (d). The dislocation barrier spacing is taken to be a function of the grain size D as described by Eq. (4), where d_o, D_o, and γ are material constants. The stress intensity range at the Stage I to Stage II transition, ΔK_T, is a function of the fatigue limit ($\Delta\sigma_e$), cyclic yield stress range and the large-crack FCG threshold (ΔK_{th}); n_1 and n_2 are the Stage I and Stage II exponents, respectively. R is the stress ratio and K_c is the fracture toughness.

The effective stress intensity range, ΔK_{eff}, is expressed as [9]

$$\Delta K_{eff} = U_P U_D U_R U_O \Delta K \tag{6}$$

where U_i is ratio of ΔK_{eff} to ΔK for individual crack closure mechanisms including plasticity- (P), deflection- (D), roughness- (R), and oxide-induced (O) closure. Analytical expressions for computing individual U_i terms, which are summarized in a recent paper [9], include Newman's formulation for treating plasticity-induced crack closure [10], Suresh's formulation for crack deflection and roughness-induced crack closure [11], as well as an oxide-wedging model.

3.2 Probabilistic Crack Initiation Modeling

The crack initiation model of Tanaka and Mura [2] was developed based on a dislocation dipole mechanism operating in a surface grain. During fatigue loading, irreversible slip occurs on parallel slip planes in a favorably oriented surface grain, producing dislocation dipoles at the ends of a double pileup whose coalescence ultimately leads to crack nucleation. Chan [3] recently extended Tanaka and Mura's model [2] to explicitly incorporate the crack size, as well as other pertinent material parameters in the response equation by considering the energetics of the fatigue crack initiation process. Specifically, the length of the incipient crack was obtained by equating the elastic strain energy released by dislocation coalescence and crack opening to the fracture energy, consisting of elastic and plastic components, required to form the crack surfaces. This formulation leads one to [3, 6]

$$(\Delta\sigma - 2Mk)N_i^{\alpha} = \left[\frac{8M^2\mu^2}{\lambda\pi(1-\nu)}\right]^{1/2}\left(\frac{h}{D}\right)\left(\frac{a}{D}\right)^{1/2} \tag{7}$$

for crack initiation at slip bands, where $\Delta\sigma$ is the stress range, M is the Taylor factor, k is the friction stress, N_i is the cycles-to-initiation, ν is Poisson's ratio, μ is shear modulus, and λ (= 0.005) is a universal constant. Eq. (7) relates the crack initiation life, N_i, to the grain size, D, the slipband width, h, and the crack half-length or depth, a. The exponent to N_i has been generalized to α where $0 < \alpha \leq 1$. The value of α is not a constant, but depends on the degree of slip irreversibility and the stacking fault energy. Expressions for crack initiation at inclusions and notches have also been developed and reported earlier [3].

3.3 Probabilistic Framework

For probabilistic modeling, the material-specific variables in Eqs. 2 and 7 are treated separately from the remaining variables. Previous studies (Chan and Torng [1], Enright and Chan [7]) suggest that some of the material-specific variables can be approximated as deterministic variables (e.g., E, s, K_c). The remaining material variables (dislocation barrier spacing d, cyclic yield stress σ'_y, fatigue ductility coefficient ε'_f) are modeled as random variables. In many instances, these material variables are all functions of the grain size D. If the non-material-specific random variables (a_i, ΔK, R) are temporarily treated as deterministic variables, Eq. (1) can be used to predict N_f scatter attributed to material variability. A general probabilistic framework has been developed to address the influences of both the material- and non-material-specific variables on the probability of fatigue fracture (Enright and Wu [12], Leverant [13], Wu *et al.* [14], Enright *et al.* [15]). The N_f scatter results shown in this report can be directly applied to this framework, allowing the designer to quantify the influences of the fundamental micromechanics variables on overall component risk. Figure 1 shows the schematics of the probabilistic framework utilized in MicroFaVa for modeling random variables.

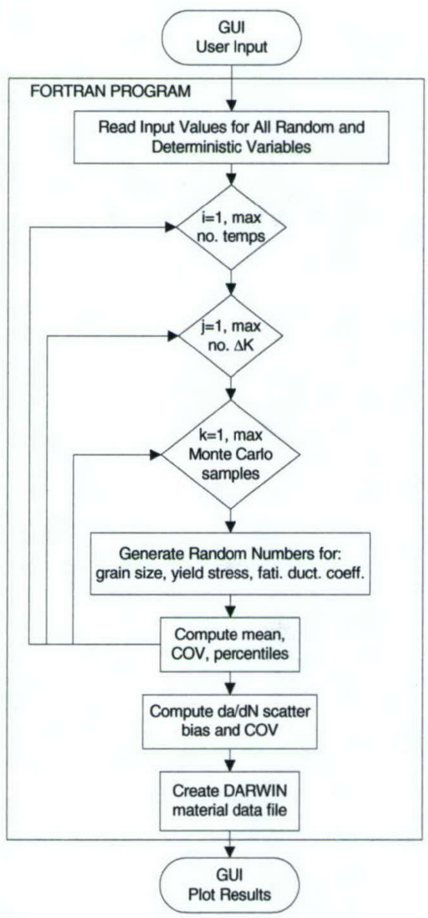


Figure 1. Schematics of the probabilistic framework in MicroFaVa for modeling material-specific random variables.

As in probabilistic crack growth modeling, material variables in Eq. (7) are treated separately from the remaining (e.g., loading) variables in probabilistic crack initiation modeling. The material specific variables include grain size (D), slipband width (h), fatigue limit (Mk), elastic properties, and Taylor factor, which is influenced by texture. The remaining variables are the stress range, cycles-to-crack initiation (N_i), and crack size (a_i) at initiation. Eq. (7) can be utilized in two ways: (1) for computing the N_i distribution for a given value of crack size at initiation, a_i, and (2) for computing the distribution of a_i for a given number of fatigue cycles. For both cases, the general probabilistic framework described by Enright et al. [15] is employed.

3.4 Model Application to Ti-6Al-4V

The probabilistic microstructure-based fatigue crack initiation and growth modeling methodology is illustrated for Ti-6Al-4V. Figure 2 shows the typical microstructure of the Ti-6Al-4V alloy, which is comprised of primary α grains and Widmanstatten $\alpha+\beta$ colonies. The volume fraction of α grain was about 60% and the average grain size was about 12 μm; both were determined using metallographic techniques. In grain size measurement, both the α grain size and the $\alpha+\beta$ colony size were treated as equivalent and fitted to one single probability density function. A log-normal distribution was used to describe the grain size distribution (D) of Ti-6Al-4V. As shown in Figure 3, this distribution provides conservative values of D compared to experimental values.

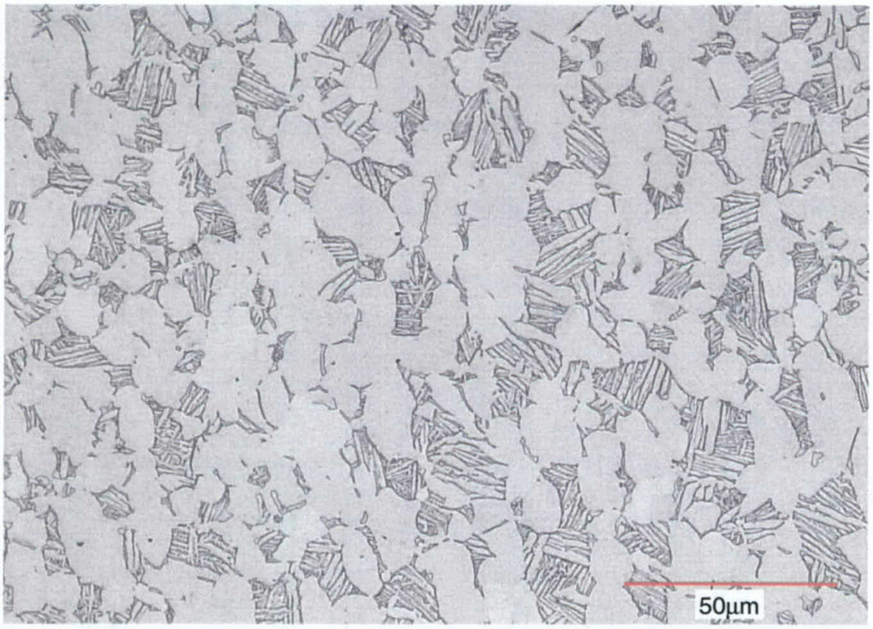


Figure 2. Microstructure of Ti-6Al-4V shows 60% primary α grain (light phase) and 40% of $\alpha+\beta$ Widmanstatten colonies.

Material constants in the FCG model were determined from FCG data for $R = 0.8$ to ensure that the FCG response was free from crack closure effects. Values for the material-related variables are indicated in Table 1. Once intrinsic material properties were obtained, the FCG model was utilized to predict deterministic *da/dN* curves for various *R* ratios by applying the crack closure model and using average values of grain size, yield stress, and fatigue ductility coefficient. The crack closure model [9] includes plasticity [10], deflection-, and roughness-induced [11] closure mechanisms, but not oxide-induced crack closure. For crack growth in Ti-6Al-4V, grain size was the dominant microstructural variable, and was modeled as a lognormal random variable (mean = 11.7 μm, standard deviation = 3.2 μm) based on grain size measurements shown in Figure 3. Cyclic yield stress σ'_y and fatigue ductility coefficient ε'_f were modeled as deterministic variables to emphasize the influence of grain size variability on *da/dN* and N_f scatter results.

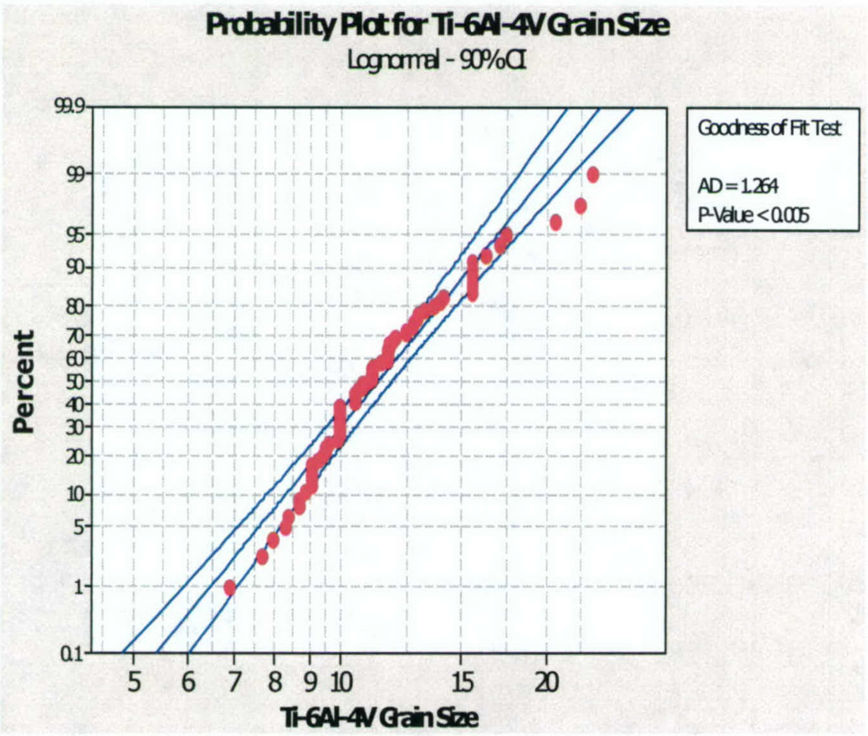


Figure 3. Grain size of Ti-6Al-4V compared against the log-normal distribution.

Table I. Values of Deterministic Material Variables for Ti-6Al-4V at 24°C used in Microstructure-based Fatigue Crack Growth Model (Eq. (2))

Variable	Description	Units	Value
E	Young's modulus	MPa	1.16×10^5
n_1	Stage I exponent	—	23.0
n_2	Stage II exponent	—	3.87
s	dislocation cell size	μm	0.25
d_o	reference dislocation barrier spacing	μm	1.0
D_o	reference grain size	μm	1.0
R	stress ratio	—	0.1
K_c	fracture toughness	$MPa\sqrt{m}$	66.7
ΔK_{th}	fatigue threshold	$MPa\sqrt{m}$	2.0
D	grain size	μm	11.7
σ'_y	cyclic yield stress	MPa	909.33
ε'_f	fatigue ductility coefficient	—	0.0389
γ	dislocation barrier spacing exponent	—	1.0

3.4.1 S-N_f Variability

The microstructure-based fatigue crack initiation and growth models were used to predict the fatigue cycles for initiating a thumb-nail crack of length $2a$ and depth c and the number of cycles for this crack to reach a critical depth. Values of material constant in the crack initiation model are presented in Table II. The computed crack initiation life, N_i, and crack growth life, N_g, for various alternating stresses, σ_a, are compared against experimental data in Figure 4. The corresponding crack length versus fatigue cycle curves of crack initiation (N_i) and crack growth (N_g) for a stress range of 552 MPa at a stress ratio R of 0.1 are presented in Figure 5. For both cases, the fatigue crack growth lives, N_g, were computed without a large-crack threshold. Variations of the N_g value were obtained when a fatigue crack growth threshold was employed. The life variation depends on the crack size at which a crack is considered to have "initiated". Different curves of crack length versus fatigue cycle were predicted for crack initiation and growth. For most cases, the transition from crack initiation to crack growth appeared to occur at a crack size of one to two grain diameters, as shown in Figures 4 and 5.

Table II. Values of Deterministic Material Variables for Ti-Al-4v at 24°C used in Microstructure-Based Fatigue Crack Initiation Model (Eq. (7))

Variable	Description	Units	Value
M	Taylor Factor	—	2
μ	Shear Modulus	MPa	4.4×10^4
ν	Poisson's Ratio	—	0.333
λ	Universal Constant	—	0.005
α	Fatigue Initiation Life Exponent	—	0.5
σ_e	Fatigue Limit (Mk)	MPa	200 - 272.5
H	Slipband Width	m	5×10^{-8}

The microstructure-based fatigue crack initiation and growth models were utilized to predict the variability of fatigue crack initiation and growth live due to grain size variations. A comparison of the predicted and observed probability density functions (PDF) for crack initiation life is shown in Figure 6, which shows that the range of initiation life values associated with the experimental data is within the values predicted by MicroFaVa.

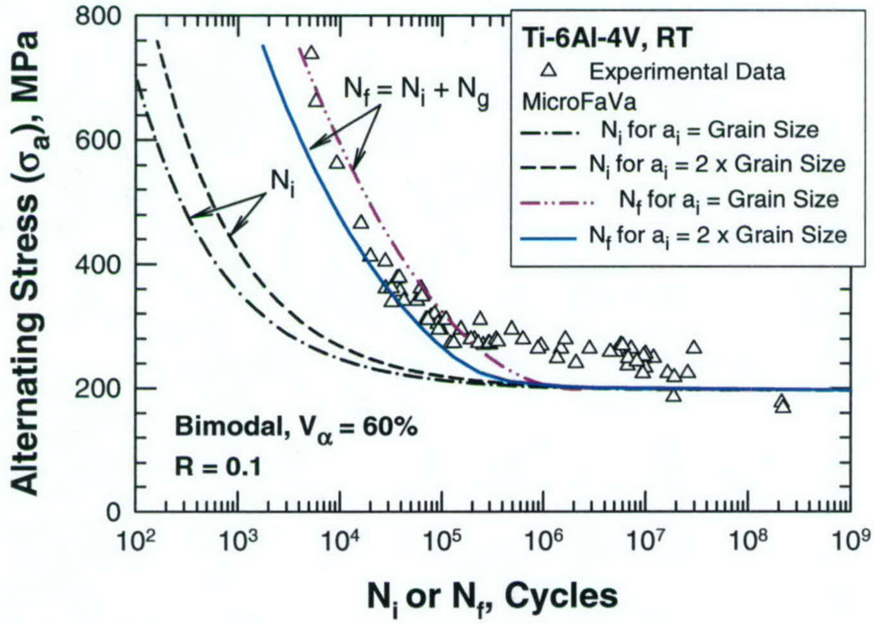


Figure 4. Predicted crack initiation life, N_i, crack growth life, N_g, and total life, N_f, compared against observed failure life for Ti-6Al-4V. Experimental data are from [17]. From Chan et al. [16].

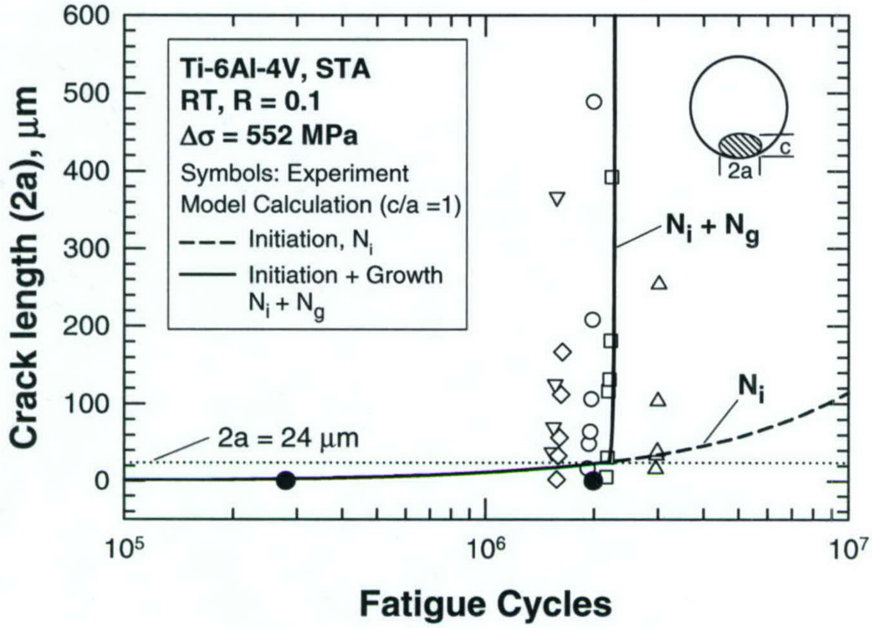


Figure 5. A comparison of predicted and measured crack lengths versus fatigue cycles for the initiation (N_i) of one grain-sized crack and its growth (N_g) to failure. Experimental data are from [17]. From Chan et al. [16].

3.4.2 Fatigue Threshold Variability

The FCG threshold model in MicroFaVa contains an intrinsic term which originates from the crack-tip cyclic slip process, and an extrinsic term which arises from a combination of plasticity-induced closure with crack deflection, asperity-induced, and oxide-induced crack closure mechanisms. In particular, the ΔK_{th} expression is given by [9]

$$\Delta K_{th} = U^{-1}\,\Delta K_{th,in} = [U_P\,U_D\,U_R\,U_O]^{-1}\,\Delta K_{th,in} \tag{8}$$

with the intrinsic threshold, $\Delta K_{th,in}$ given by [9]

$$\Delta K_{th,in} = 0.1\left[\frac{ME}{\sigma_{ys}}\right]^{1/2} Eb^{1/2} \tag{9}$$

where b is the magnitude of the Burgers vector. The proposed model was applied to compute the ΔK_{th} for Ti-6Al-4V for R values ranging from –1 to 1 and the results are presented in Figure 7. For these calculations, $\Delta K_{th,in}$ ranges from 1.2 MPa√m to 2.0 MPa√m. Most of the crack closure was contributed by crack-wake plasticity. Figure 7 shows a comparison of model calculations against experimental data of Ti-6Al-4V from the HCF program [18] at Air Force Research Laboratory (AFRL), Marci et al. [19, 20], and Boyce and Ritchie [21].

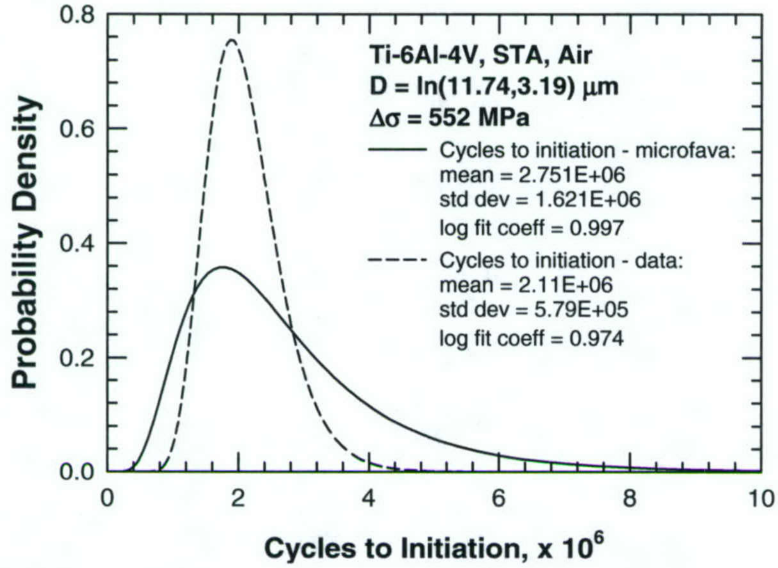


Figure 6. Measured PDF for cycles-to-initiation compared against MicroFaVa model prediction based on measured grain-size distribution. From Chan et al. [16].

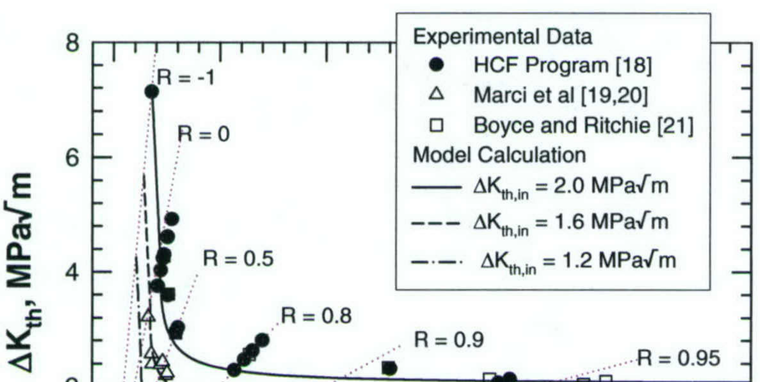


Figure 7. Comparison of model predictions against measured ΔK_{th} for Ti-6Al-4V as a function of K_{max}. From Chan [9].

The Ti-6Al-4V alloy studied by Boyce and Ritchie [21] were identical to those used in the HCF program; hence, there was good agreement between these two sets of ΔK_{th} data. For these two sets of data, $\Delta K_{th,in}$ = 2 MPa√m, it was correctly predicted by the intrinsic threshold model, Eq. (9). The increase in ΔK_{th} at $R \leq 0.8$ was caused entirely by crack closure mechanisms. The lower $\Delta K_{th,in}$ value (1.2 MPa√m) for the Ti-6Al-4V material studied by Marci et al. [19, 20] was predicted from Eq. (9) using a Taylor factor of $M \approx 2$. This value of M appeared to give the lower bound for $\Delta K_{th,in}$. Again, the increase in ΔK_{th} at R < 0.5 was entirely due to crack closure mechanisms. Thus, the variation of $\Delta K_{th,in}$ from 1.2 MPa√m to 2 MPa√m could arise from microstructural effects such as texture (different values of M), yield stress, and cell formation. On the other hand, the variation of ΔK_{th} at low R ratio ($R < 0.5$) is likely caused by crack closure.

3.4.3 Crack Growth Rate Variability

Crack growth rate (mean and 1%/99% confidence limit) values for $R = 0.1$ predicted using Eq. (2) are compared against experimental data [21-24] in Figure 8. A total of 67 sets of *da/dN* data of Ti-6Al-4V of the same or equivalent material and microstructure are presented in Figure 8. Experimental *da/dN* data at selected ΔK values were also analyzed to obtain probability densities. These results are compared against probability densities and coefficient of variation (COV) of predicted crack growth rate at selected ΔK values in Figure 9. It can be observed from Figure 9(a) that the PDF values based on the experimental data are bound by the microstructure-based PDF values for most of the ΔK values considered. Figure 9(b) shows that the predicted COV is about 0.54 - 0.56 over the ΔK range of 3 MPa√m to 90 MPa√m. The two largest values of the experimentally determined COV are 0.45 at ΔK = 15 MPa√m and 0.48 at ΔK = 45 MPa√m. The larger discrepancy at ΔK values in the range of 18 – 30 MPa√m is due to insufficient experimental data in that crack growth regime.

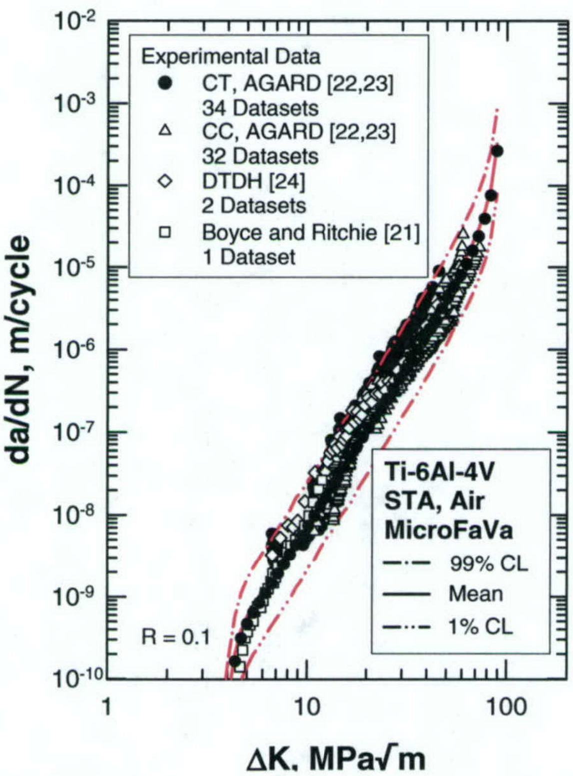
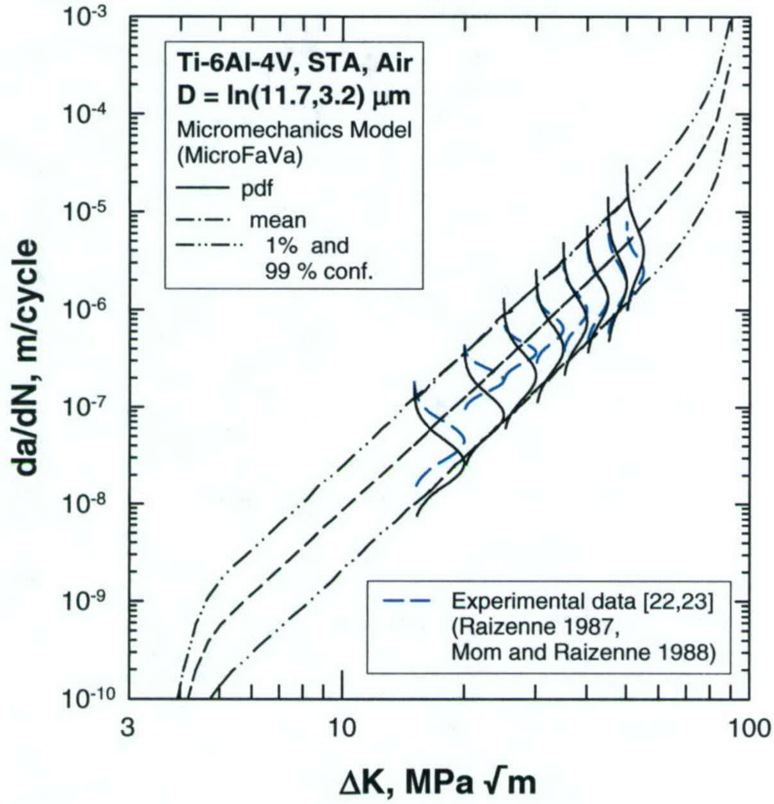
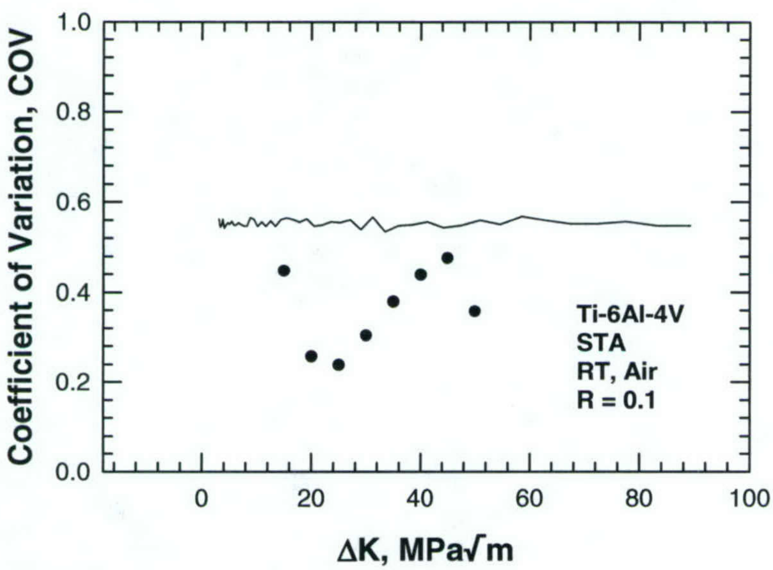


Figure 8. Measured *da/dN* data compared against model predictions based on a log-normal grain size distribution [16].



(a)



(b)

Figure 9. Comparison of computed crack growth rate predictions, probability density functions, and coefficient of variation (COV) with experimental data for $R = 0.1$ at 24°C: (a) da/dN and probability density functions, and (b) coefficient of variation of da/dN.

3.4.4 Crack Growth Life Variability

Computational and experimental *da/dN* values were applied to the life prediction of a 10 cm × 10 cm Ti-6Al-4V plate with material properties indicated in Table 1. A uniform stress range of 600 MPa was applied to the plate at a stress ratio, *R*, of 0.1 and an initial crack (0.035 cm × 0.035 cm) was placed at one of the corners. Crack growth life was computed using probabilistic fracture mechanics software (DARWIN® 2004 [8]) using: (1) tabular *da/dN* values based on Eq. (2), and (2) *da/dN* slope and intercept constants based on linear and bilinear curve fits of experimental data from the literature (Raizenne 1987 [22], Mom and Raizenne 1988 [23]). The results are shown in Figure 10. It can be observed that all of the predicted crack growth life values based on the experimental *da/dN* data fall within the 5% and 95% confidence limits based on life values associated with the computational model (Eq. (2)). The corresponding computed and observed probability density of crack propagation life are compared in Figure 11, which shows that the predicted mean is in good agreement with the experimental data. On the other hand, the predicted variability is larger than experimental observations and is, thus, more conservative. As shown in Figure 11, the observed COV is about 0.23 while the predicted COV is 0.57. The observed COV is lower partly because of the sampling size and partly because the COVs associated with curve-fitting of individual da/dN datasets have not been included in the computation of the experimental COV. The observed COV is expected to approach the predicted COV as the sampling size increases and the COVs of individual da/dN datasets are taken into account. Additional FCG life computations for $\Delta\sigma = 552$ MPa indicates that the predicted COV is independent of the applied stress and depends only on the grain size distribution since stress variations are not considered in these calculations.

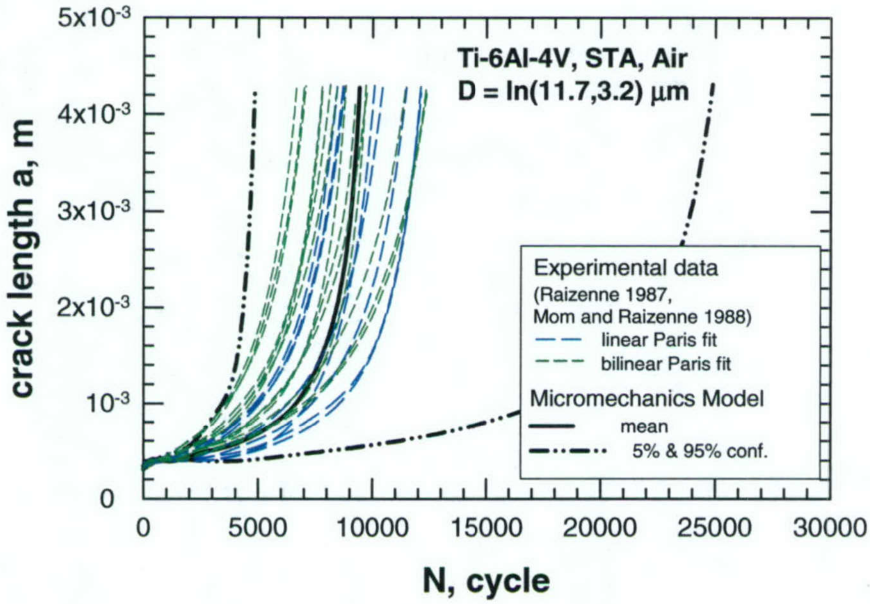


Figure 10. Comparison of predicted crack growth life values based on microstructure-based computational model and experimental data *da/dN* results [22, 23] for $R = 0.1$ at 24°C [16].

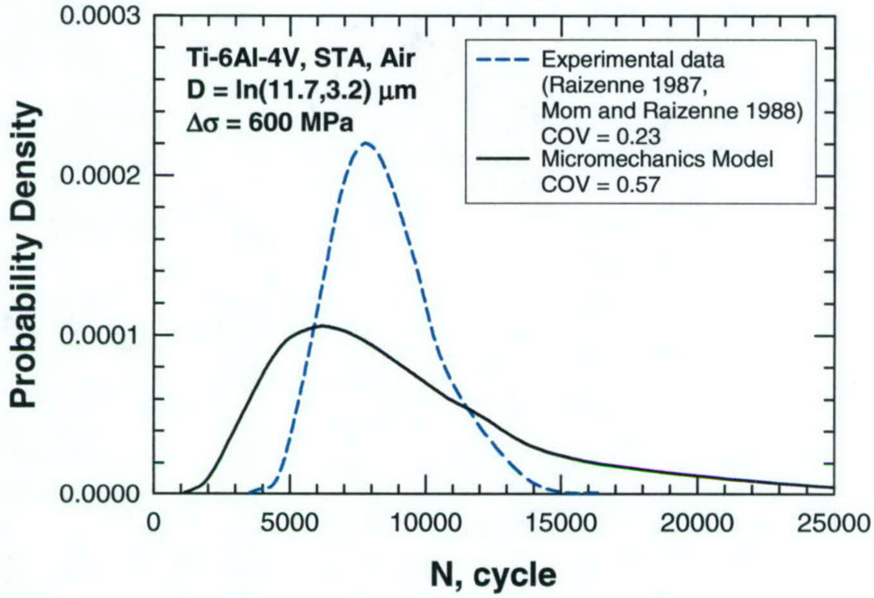
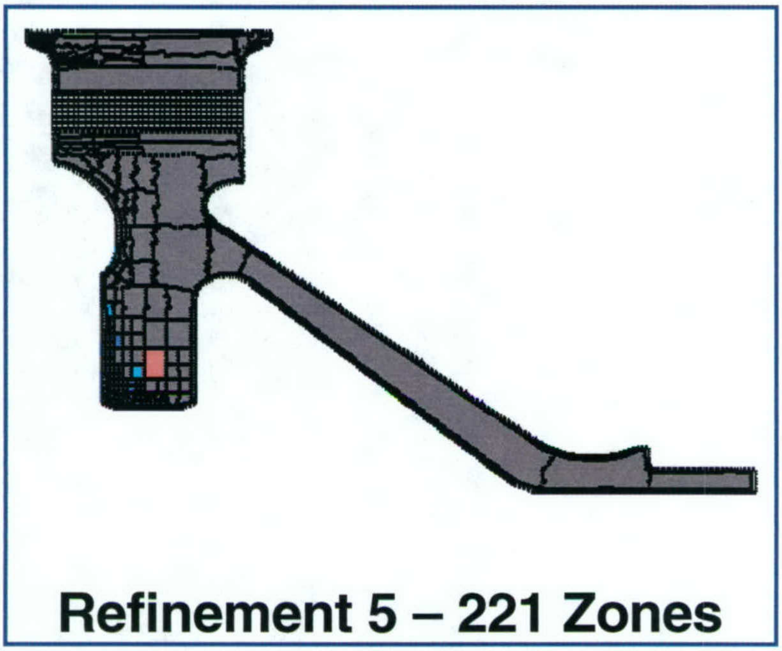


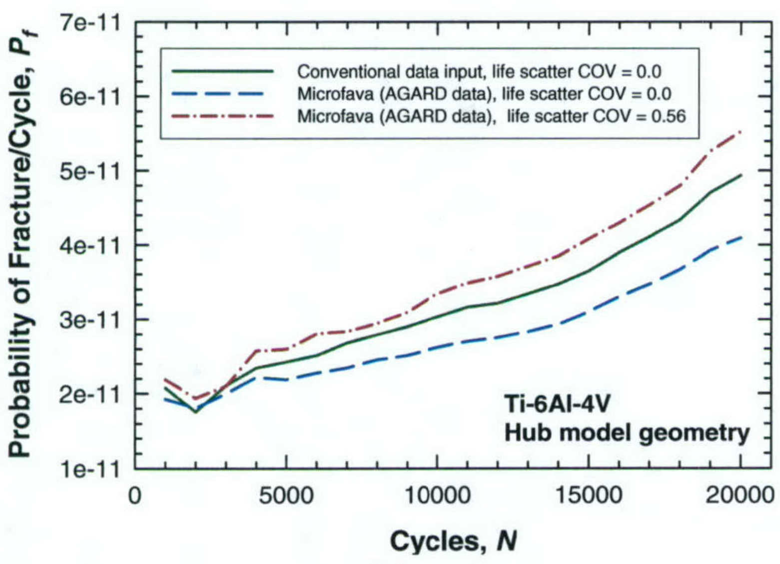
Figure 11. Comparison of computed and observed probability density of FCG lives based on microstructure-based computational model and experimental data *da/dN* results [22, 23] for $R = 0.1$ at 24°C.

3.5 Application to Probabilistic Life Prediction of Titanium Components

Two example problems were solved to validate the MicroFaVa prediction and its integration with DARWIN®. For the first validation case, the calibration problem of a fictitious titanium rotor disk subjected to a single inertial load in FAA Advisory Circular AC33.14-1 [25] and an empirically derived hard alpha distribution [13] as the initial crack size distribution were used to assess the MicroFaVa/DARWIN® *da/dN* and life predictions. Essentially identical results were obtained by the current methodology and those reported in the FAA Circular. In the second validation, MicroFaVa and DARWIN® were used to analyze the probability of fatigue fracture of a representative Ti rotor design. As in the first problem, the initial crack size was described by the distribution of the hard alpha particle size and a power-law FCG relation was used. Figure 12(a) shows the rotor disk design divided into 221 zones after 5 zone refinements. The predicted probability of fracture computed on the basis of conventional (experimental *da/dN* data) material input and MicroFaVa input are compared in Figure 12(b). It should be noted that the results based on the conventional data input did not consider the coefficient of variation (COV) of *da/dN*. Without considering the COV, the DARWIN® prediction using MicroFaVa input is slightly less conservative than that using the conventional input. The ability of MicroFaVa to predict the COV in addition to the mean *da/dN* allows one to quantify the increase in the probability of fracture due to *da/dN* variation. As shown in Figure 12(b), the predicted probability of fracture is increased slightly above the conventional method line when the COV predicted from MicroFaVa is incorporated into the DARWIN® design analysis. These computations illustrate that MicroFaVa is a viable methodology for predicting fatigue variability due to microstructural variations and is highly compatible with probabilistic design and life-prediction methods.



(a)



(b)

Figure 12. Analysis of a Ti rotor design using MicroFaVa and DARWIN®: (a) hub geometry with the critical region in red, and (b) computed probability of fracture [16].

4.0 CONCLUSIONS

In this report, the development of a probabilistic microstructure-based crack initiation and growth model was summarized and the model capability was illustrated for life prediction of Ti-6Al-4V. It was shown that the microstructure-based S-N_f and *da/dN* simulation results are in agreement with experimental data for the range of values considered in this study. Fatigue life variability in Ti-6Al-4V appears to originate, at least partly if not totally, from microstructural variability in the form grain size variations. In addition, the microstructure-based models appear to provide reasonable estimates of crack growth life and total life variability when compared with life values based on experimental *da/dN* and S-N_f data. Application of the probabilistic fatigue model to a Ti alloy rotor design illustrates that the proposed model is capable of predicting the confidence bounds of the fatigue life and can significantly reduce the database requirement used to define fatigue life variability.

5.0 LIST OF ACCOMPLISHMENTS

The accomplishments achieved in this program are as follows:

1. The development of a set of physics-based fatigue models for predicting fatigue crack initiation and growth in structural alloys. This suite of fatigue models allows predictions of FCG rate (da/dN versus ΔK) response, stress-life (S-N_f) data, FCG thresholds for small and large cracks, and dual fatigue limits for crack initiation and crack growth.

2. The formulation of a probabilistic framework of treating fatigue life variability due to variations of microstructure. This formulation enables prediction of the mean and the variance of fatigue life including the worst-case limit on the basis of the probability density distribution of the pertinent microstructural length scale or other relevant material variables.

3. Implementation of physics-based fatigue crack initiation and growth models in the probabilistic framework to form a probabilistic micromechanical code dubbed MicroFaVa for predicting variability in initial crack size, fatigue crack growth rate, and ultimately fatigue crack initiation, crack growth life, as well as the total life and their confidence bounds due to material variability or uncertainties in material properties.

4. The integration of MicroFaVa with a probabilistic design and life-prediction code named DARWIN® (Damage Assessment of Reliability With INspection) and the application of the integrated methodology for probabilistic design and lifing of a Ti rotor.

5. An extensive and systematic assessment of the predictive capability of the physics-based fatigue models by comparisons against a large experimental database

of fatigue life data and fatigue crack growth rate data of a Ni-based alloy and a Ti-based alloy.

6. Verification and validation of the integrated probabilistic design and lifing methodology by applying the computational approach to two benchmark problems with known solutions. The utility of the computed material input has been successfully demonstrated by one to one comparisons against the conventional method based on empirical data input.

7. The application of the probabilistic micromechanical code to elucidate the influence of microstructural variation on the propagation and arrest of grain-sized small cracks, the probability density function of small-crack thresholds, as well as the occurrence of dual fatigue limits for crack initiation and growth.

8. The development of fundamental understandings on several microstructure/fatigue resistance relationships: (i) the dependence of the intrinsic threshold on the planarity of slip and dislocation cell formation, (iii) the occurrence of dual fatigue thresholds and dual fatigue limits, (iii) fatigue life variation resulting from difference in the slip morphology and enhanced fatigue crack initiation life by dislocation cell formation, and (iv) dependence of FCG rate on dislocation density at the crack tip.

6.0 LIST OF PERSONNEL SUPPORTED

The personnel supported during the three-year duration of this program are listed as follows:

1. Dr. Kwai. S. Chan, Institute Scientist, Materials Engineering Department, Mechanical and Materials Engineering Division, Southwest Research Institute.

2. Dr. Michael P. Enright, Principal Engineer, Materials Engineering Department, Mechanical and Materials Engineering Division, Southwest Research Institute.

3. Dr. Jung S. Kong, Post-doctoral Researcher, Materials Engineering Department, Mechanical and Materials Engineering Division, Southwest Research Institute. Dr. Kong is currently an Assistant Professor in the Department of Civil Engineering at Korea University, Souel, Republic of Korea.

4. Dr. Yi-der Lee, Principal Engineer, Materials Engineering Department, Mechanical and Materials Engineering Division, Southwest Research Institute.

5. Dr. David L. Davidson, Consultant, Materials Engineering Department, Mechanical and Materials Engineering Division, Southwest Research Institute.

6. Dr. Ronald L. Bagley, Professor, Department of Mechanical Engineering and Biomechanics, University of Texas at San Antonio, San Antonio, Texas.

7. Mr. Simeon Fitch, Computer Software Programmer, Mustardseed Software, Virginia.

7.0 LIST OF PUBLICATIONS

The publications supported by this program are listed as follows:

1. "Physically Based Models for Predicting Fatigue Life Variability in Ni-Based Superalloys," K. S. Chan and M. P. Enright, Modeling the Performance of Engineering Structure Materials III, edited by T. Srivatsan, D. Lesuer, and E. Taleff, TMS, Warrendale, PA, 2002, pp. 135-142.

2. "Application of Microstructure-Based Fatigue Models to Component Life Prediction," K. S. Chan and M. P. Enright, Fatigue 2003, edited by M. R. Bache, P. A. Blackmore, J. Draper, J. H. Edwards, P. Roberts, and J. R. Yates, Engineering Integrity Society, Sheffield, U.K., 2003, pp. 39-48.

3. "Extension of a Microstructure-Based Fatigue Crack Growth Model for Predicting Fatigue Life Variability," by M. P. Enright and K. S. Chan, Proceedings of ASTM Symposium on Probabilistic Aspects of Life Prediction, edited by W.S. Johnson and B.M. Hillberry, ASTM STP 1450, ASTM International, West Conshohocken, PA, 2004, pp. 87 – 103. Journal of ASTM International, Vol. 1, 2004, N0. 8, September 2004, Paper JAI11566.

4. "Variability of Large-Crack Fatigue Crack Growth Thresholds In Structural Alloys," *Metallurgical and Materials Transactions A*, Vol. 35A, 2004, pp. 3721 - 3735.

5. "MicroFaVa: A Micromechanical Code for Predicting Fatigue Life Variability," K.S. Chan, M.P. Enright, and J.S. Kung, ***Materials Damage Prognosis***, James M. Larsen, Leo Christodoulou, Jeffrey R. Calcaterra, Michael L. Dent, Mark M. Derriso, William J. Hardman, J. Wayne Jones, and Stephan M. Russ (eds.), TMS, Warrendale, PA, 2004 (in press).

6. "A Probabilistic Micromechanical Code for Predicting Fatigue Life Variability: Model Development and Application," K.S. Chan and M.P. Enright, Proceedings of ASME Turbo Expo 2005 Power for Land, Sea, & Air, Paper GT2005-68983, June 6-9, 2005, Reno-Tahoe, Nevada (In Review).

7. "Probabilistic Micromechanical Modeling of Fatigue Life Variability in an $\alpha + \beta$ Ti-Alloy," K. S. Chan and M. P. Enright, *Metallurgical and Materials Transactions A*, 2004 (In Review).

8. "Variability of Fatigue Life in Two-Phase Alloys," K.S. Chan, Y-D. Lee, and M. P. Enright, Proceedings of Computational Aspects of Mechanical Properties of

Materials, 2005 TMS Annual Meeting, Feb 11-17, 2005, San Francisco, CA, *Metallurgical and Materials Transactions A*, 2004 (In Preparation).

8.0 LIST OF PRESENTATIONS

The presentations supported by this program are listed as follows:

1. "Physically Based Fatigue Models for Predicting Fatigue Life Variability in Ni-Based Superalloys," K. S. Chan and M. P. Enright, Symposium on Modeling the Performance of Engineering Structure Materials III, 2002 AMS/TMS Materials Week, Columbus, OH, October 6 –10, 2002.

2. "Physically-Based Life-Prediction Models for Applications in Engine Integrity Prognosis," K. S. Chan, TMS Annual Meeting, San Diego, CA, March 2-6, 2003.

3. "Extension of a Microstructure-Based Fatigue Crack Growth Model for Predicting Fatigue Life Variability," by M. P. Enright and K. S. Chan, Presented at ASTM Symposium on Probabilistic Aspects of Life Prediction, Miami, FL, November 6-7, 2002.

4. "Application of Microstructure-Based Fatigue Models to Component Life Prediction," K. S. Chan and M. P. Enright, The Engineering Integrity Society Fatigue 2003 – Fatigue & Durability Assessment of Materials, Components and Structures, Queen's College, Cambridge, UK, April 7 –9, 2003.

5. "MicroFaVa: A Micromechanical Code for Predicting Fatigue Life Variability," K.S. Chan, M.P. Enright, and J.S. Kung, Presented at AFOSR US-Korea Workshop 2, Jeju City, republic of Korea, may 11-13,2004.

6. "Application of a Microstructure-Based fatigue Crack Growth Model to Probabilistic Life Prediction," M.P. Enright and K.S. Chan, The Ninth ASCE Specialty Conference on Probabilistic Mechanics and Structural Reliability," Sandia National Laboratories, Albuquerque, NM, July 26-28, 2004.

7. "MicroFaVa: A Micromechanical Code for Predicting Fatigue Life Variability," K.S. Chan, M.P. Enright, and J.S. Kung, Presented at TMS Symposium on Materials Damage Prognosis, 2005 TMS Materials Week, New Orleans, LA, September 26-30, 2004.

8. "A Probabilistic Micromechanical Code for Predicting Fatigue Life Variability: Model Development and Application," K.S. Chan and M.P. Enright, ASME Turbo Expo 2005 Power for Land, Sea, & Air, Paper GT2005-68983, Reno-Tahoe, Nevada, June 6-9, 2005.

9. "Variability of Fatigue Life in Two-Phase Alloys," K.S. Chan, Y-D. Lee, and M. P. Enright, Symposium on Computational Aspects of Mechanical Properties of Materials, 2005 TMS Annual Meeting, San Francisco, CA, Feb 11-17, 2005

9.0 TRANSITIONS AND AWARDS

9.1 Transitions

The technology developed in this program has been incorporated into DARWIN and transferred to the USAF DUST program (Contract No. F33615-03-2-5203) with SwRI. The Program Manager of the DUST program is Dr. Patrick Golden (phone: (937) 255-5438) at Air Force Research Laboratory, WPAFB, Dayton, OH.

The probabilistic micromechanics-based life methodology is in the process of being transferred to a DARPA-supported program entitled "A Revolutionary Smart Materials Approach to Structural Health Monitoring and Progress" (Contract No. HR0011-04-0004; Dr. Leo Christodoulu, Program Manager; (703) 696-2374) at SwRI and an AFOSR program entitled "Vehicle Health Monitoring" (Contract No. FA95500410254, Dr. Thomas Kim, Program Manager; (703) 696-7312) at University of Texas at San Antonio.

9.2 Awards Received

No award was received during the reporting period.

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